

Isophorone

78-59-1 | DTXSID8020759

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 7.69e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.33e-01

Confidence level: 8.15e-01

Nearest Neighbors from the Training Set

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1-Nitrocyclohex-1-ene

Measured: 4.37e-11

Predicted: 3.80e-11

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11

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(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11

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4-Methylcyclohex-3-en-1-one

Measured: 1.29e-10

Predicted: 3.70e-11

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6-Methyl-5-hepten-2-one

Measured: 1.57e-10

Predicted: 1.41e-10